An Approach to Semantic Chemistry

Chemantics

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Chief Scientific Officer

Chemantics - Overview

Chemantics – a OSTHUS Company

- German company with global presence
- Highly experienced in delivering R&D solutions and consulting expertise

OSTHUS
success with R&D

Chemistry Tools in partnership with

ChemAxon

Data integration Partner

ONTOFORCE

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Chemical Structures in R&D

The Chemantics Infrastructure integrates public and proprietary data across R&D domains based on chemical structures and reactions.

Overview

Competitive Intelligence
- IP Capture
- Patent Analysis

Commercial Compounds
- Proprietary Compounds
- Vendor Catalogs

Document Analytics
- Scientific Publications
- Proprietary Documents

Aggregated Data Sources
- Doman Specific DBs
- Reaction Databases

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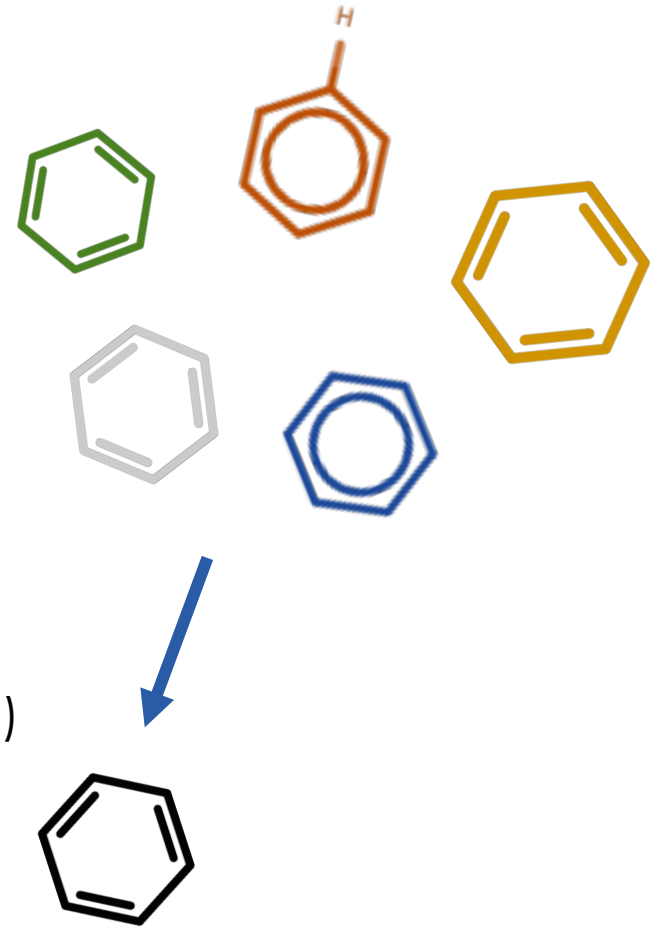
The Chemantic Process

Analysis

- Standardize
- Validate
- Annotate
- Build chemantic graph
- Prepare structure search

Key Features

- Data provenance
- 8 inferred chemical species
- Classification Ontology
  (~600 features, functional groups, etc.)
- Sort Index
- Universal Resource Identifier



Process

analyze

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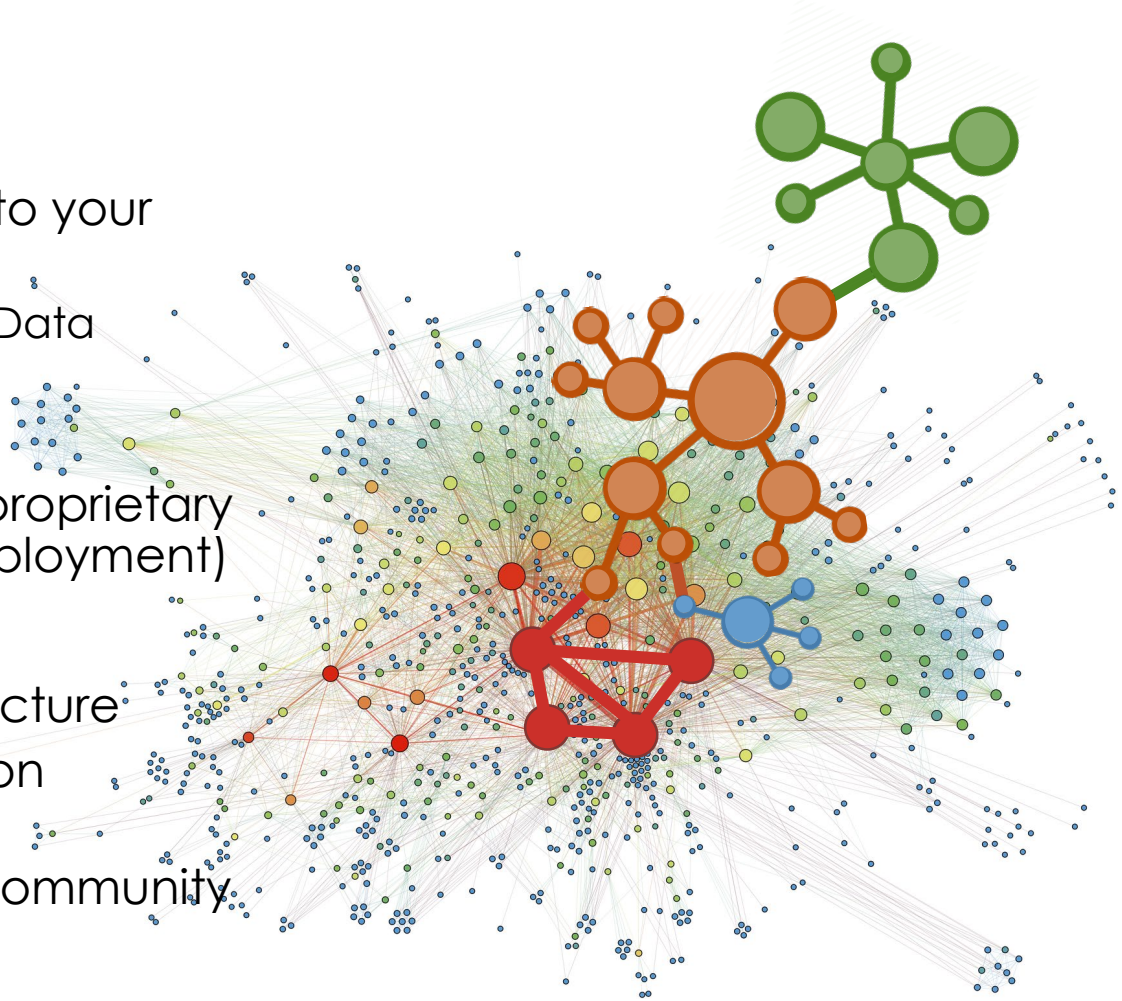
The Chemantic Process

Ingestion

- Integrate data set into your system of choice!
  - Reference Master Data
  - Semantic UI
  - Data Sharing
- Clear separation of proprietary and public data (deployment)

Key Features

- Rest Protocol Architecture
- Continuous integration capabilities
- Transparent to user community



Process

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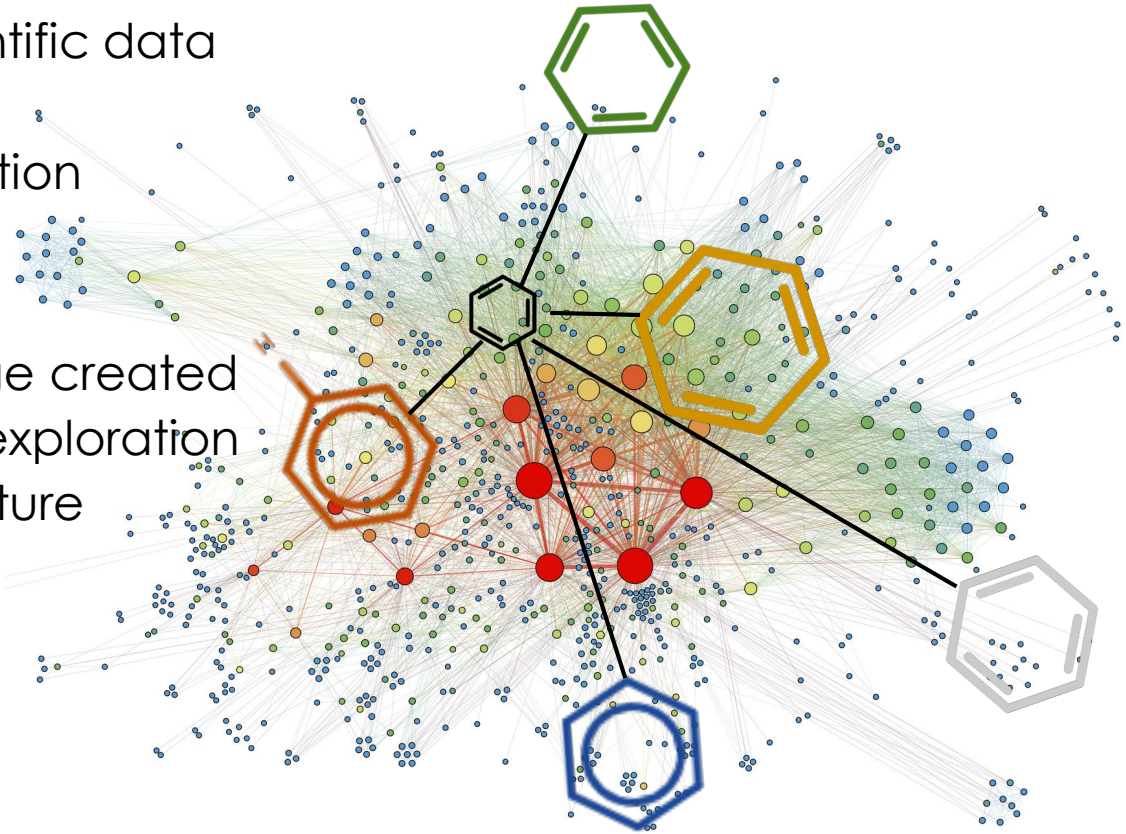
The Chemantic Process

Exploration

- Holistic view on scientific data
- Tool independent
- Feature and Annotation browsing

Key Features

- Additional knowledge created
- Cross domain data exploration
- 1 stop shop architecture



Process

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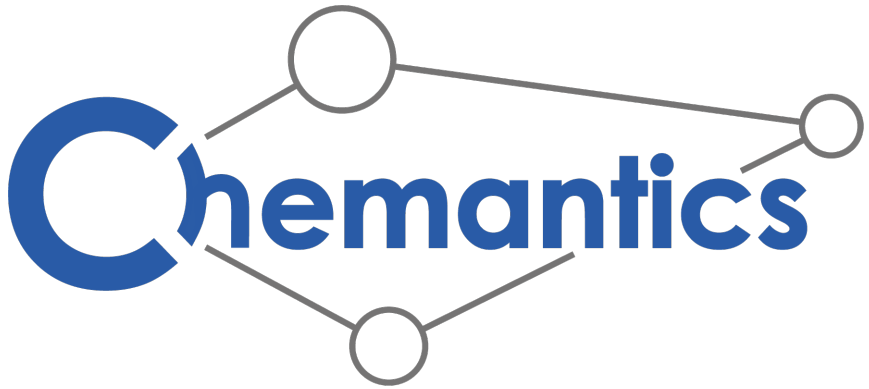
Thank you!